

1-Heptene

Other names:	1-C7H14 1-n-Heptene HEPTYLENE N-HEPT-1-ENE NSC 74130 hept-1-ene heptene-1 «alpha»-Heptylene Â«alphaÂ»-Heptylene
Inchi:	InChI=1S/C7H14/c1-3-5-7-6-4-2/h3H,1,4-7H2,2H3
InchiKey:	ZGEGCLOFRBLKSE-UHFFFAOYSA-N
Formula:	C7H14
SMILES:	C=CCCCCC
Mol. weight [g/mol]:	98.19
CAS:	592-76-7

Physical Properties

Property code	Value	Unit	Source
af	0.3580		KDB
aigt	533.15	K	KDB
ap	300.350	K	KDB
chl	-4657.00 ± 0.75	kJ/mol	NIST Webbook
chl	-4650.98 ± 0.79	kJ/mol	NIST Webbook
chl	-4658.30 ± 1.20	kJ/mol	NIST Webbook
dm	0.30	debye	KDB
fl	1.00	% in Air	KDB
fpo	269.26	K	KDB
gf	95.88	kJ/mol	KDB
hcg	4658.34	kJ/mol	KDB
hcn	4350.272	kJ/mol	KDB
hf	-63.00	kJ/mol	NIST Webbook
hf	-63.70	kJ/mol	NIST Webbook
hf	-62.34	kJ/mol	KDB
hf	-62.30	kJ/mol	NIST Webbook
hfl	-98.37 ± 0.88	kJ/mol	NIST Webbook
hfl	-97.70 ± 0.63	kJ/mol	NIST Webbook
hfl	-97.00 ± 1.20	kJ/mol	NIST Webbook

hfus	12.61	kJ/mol	Joback Method
hvap	35.70	kJ/mol	NIST Webbook
ie	9.44 ± 0.00	eV	NIST Webbook
ie	9.30 ± 0.10	eV	NIST Webbook
ie	9.27 ± 0.02	eV	NIST Webbook
ie	9.38 ± 0.05	eV	NIST Webbook
ie	9.34 ± 0.08	eV	NIST Webbook
log10ws	-3.73		Aqueous Solubility Prediction Method
log10ws	-3.73		Estimated Solubility Method
logp	2.753		Crippen Method
mcvol	105.190	ml/mol	McGowan Method
pc	2920.00 ± 40.00	kPa	NIST Webbook
pc	2920.00	kPa	KDB
rhoc	235.65 ± 3.93	kg/m3	NIST Webbook
rinpol	688.60		NIST Webbook
rinpol	689.00		NIST Webbook
rinpol	688.00		NIST Webbook
rinpol	689.00		NIST Webbook
rinpol	688.10		NIST Webbook
rinpol	688.90		NIST Webbook
rinpol	682.00		NIST Webbook
rinpol	682.60		NIST Webbook
rinpol	689.00		NIST Webbook
rinpol	692.00		NIST Webbook
rinpol	689.00		NIST Webbook
rinpol	689.00		NIST Webbook
rinpol	690.00		NIST Webbook
rinpol	693.90		NIST Webbook
rinpol	693.90		NIST Webbook
rinpol	693.80		NIST Webbook
rinpol	693.80		NIST Webbook
rinpol	693.80		NIST Webbook
rinpol	693.80		NIST Webbook
rinpol	690.00		NIST Webbook
rinpol	689.00		NIST Webbook
rinpol	688.80		NIST Webbook
rinpol	689.20		NIST Webbook
rinpol	689.60		NIST Webbook
rinpol	690.00		NIST Webbook
rinpol	690.00		NIST Webbook
rinpol	690.90		NIST Webbook
rinpol	687.30		NIST Webbook
rinpol	687.70		NIST Webbook

rinpol	688.00	NIST Webbook
rinpol	688.40	NIST Webbook
rinpol	688.80	NIST Webbook
rinpol	689.20	NIST Webbook
rinpol	697.00	NIST Webbook
rinpol	684.00	NIST Webbook
rinpol	681.80	NIST Webbook
rinpol	682.20	NIST Webbook
rinpol	681.90	NIST Webbook
rinpol	681.50	NIST Webbook
rinpol	683.00	NIST Webbook
rinpol	682.00	NIST Webbook
rinpol	684.50	NIST Webbook
rinpol	682.90	NIST Webbook
rinpol	684.90	NIST Webbook
rinpol	683.60	NIST Webbook
rinpol	684.90	NIST Webbook
rinpol	682.00	NIST Webbook
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rinpol	684.00	NIST Webbook
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rinpol	689.40	NIST Webbook
rinpol	682.10	NIST Webbook
rinpol	682.00	NIST Webbook
rinpol	685.00	NIST Webbook
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rinpol	683.00	NIST Webbook
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rinpol	689.00	NIST Webbook
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rinpol	685.00	NIST Webbook

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rinpol	688.00	NIST Webbook
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rinpol	689.40	NIST Webbook
rinpol	690.90	NIST Webbook
rinpol	689.30	NIST Webbook
rinpol	690.00	NIST Webbook
rinpol	688.00	NIST Webbook
rinpol	689.00	NIST Webbook
rinpol	689.40	NIST Webbook
rinpol	686.00	NIST Webbook
rinpol	689.01	NIST Webbook
rinpol	689.10	NIST Webbook
rinpol	689.22	NIST Webbook
rinpol	691.74	NIST Webbook
rinpol	691.87	NIST Webbook
rinpol	691.94	NIST Webbook
rinpol	685.00	NIST Webbook
rinpol	699.00	NIST Webbook
rinpol	688.00	NIST Webbook
rinpol	685.00	NIST Webbook
rinpol	681.30	NIST Webbook
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rinpol	687.00	NIST Webbook
rinpol	689.00	NIST Webbook
rinpol	690.00	NIST Webbook
rinpol	693.00	NIST Webbook
rinpol	686.00	NIST Webbook
rinpol	689.00	NIST Webbook
rinpol	687.00	NIST Webbook
rinpol	683.76	NIST Webbook
rinpol	689.00	NIST Webbook
rinpol	686.00	NIST Webbook
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rinpol	689.00	NIST Webbook
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rinpol	690.00	NIST Webbook
rinpol	691.80	NIST Webbook
rinpol	692.00	NIST Webbook
rinpol	692.00	NIST Webbook
rinpol	681.00	NIST Webbook
rinpol	689.00	NIST Webbook
rinpol	688.00	NIST Webbook
rinpol	683.00	NIST Webbook
rinpol	682.30	NIST Webbook
rinpol	681.80	NIST Webbook
rinpol	688.70	NIST Webbook
rinpol	688.60	NIST Webbook
rinpol	688.70	NIST Webbook
rinpol	686.00	NIST Webbook
rinpol	685.90	NIST Webbook
rinpol	681.00	NIST Webbook
rinpol	683.00	NIST Webbook
rinpol	685.00	NIST Webbook
rinpol	681.10	NIST Webbook
rinpol	688.60	NIST Webbook
rinpol	695.00	NIST Webbook
rinpol	689.00	NIST Webbook
ripol	740.00	NIST Webbook
ripol	740.00	NIST Webbook
ripol	736.00	NIST Webbook
ripol	751.00	NIST Webbook
ripol	751.00	NIST Webbook
ripol	741.00	NIST Webbook
ripol	747.00	NIST Webbook
ripol	748.00	NIST Webbook
ripol	749.00	NIST Webbook
ripol	731.00	NIST Webbook
ripol	747.70	NIST Webbook

ripol	747.30		NIST Webbook
ripol	749.00		NIST Webbook
ripol	747.30		NIST Webbook
ripol	747.70		NIST Webbook
ripol	749.00		NIST Webbook
ripol	750.00		NIST Webbook
sl	328.90	J/molxK	NIST Webbook
sl	327.65	J/molxK	NIST Webbook
tb	366.79	K	KDB
tc	537.23 ± 0.05	K	NIST Webbook
tc	537.30	K	KDB
tc	537.30 ± 0.40	K	NIST Webbook
tf	153.40	K	KDB
tf	153.69	K	Aqueous Solubility Prediction Method
tt	154.30 ± 0.05	K	NIST Webbook
tt	153.40 ± 0.20	K	NIST Webbook
tt	153.89 ± 0.05	K	NIST Webbook
vc	0.409	m ³ /kmol	NIST Webbook
vc	0.409	m ³ /kmol	KDB
zc	0.2673330		KDB
zra	0.26		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	180.50	J/molxK	356.24	Joback Method
cpg	202.58	J/molxK	411.88	Joback Method
cpg	241.81	J/molxK	523.16	Joback Method
cpg	232.58	J/molxK	495.34	Joback Method
cpg	222.98	J/molxK	467.52	Joback Method
cpg	191.75	J/molxK	384.06	Joback Method
cpg	212.98	J/molxK	439.70	Joback Method
cpl	212.84	J/molxK	295.10	NIST Webbook
cpl	211.79	J/molxK	298.15	NIST Webbook
dvisc	0.0002312	Paxs	356.24	Joback Method
dvisc	0.0005794	Paxs	261.56	Joback Method
dvisc	0.0002959	Paxs	324.68	Joback Method
dvisc	0.0003993	Paxs	293.12	Joback Method
dvisc	0.0009312	Paxs	230.01	Joback Method
dvisc	0.0017402	Paxs	198.45	Joback Method

dvisc	0.0041197	Paxs	166.89	Joback Method
hfust	12.64	kJ/mol	154.30	NIST Webbook
hfust	12.66	kJ/mol	153.40	NIST Webbook
hfust	12.66	kJ/mol	154.30	NIST Webbook
hvapt	31.09	kJ/mol	366.80	KDB
hvapt	33.90	kJ/mol	347.00	NIST Webbook
hvapt	35.30	kJ/mol	306.50	NIST Webbook
hvapt	35.93	kJ/mol	300.00	NIST Webbook
hvapt	35.90	kJ/mol	283.50	NIST Webbook
hvapt	34.60	kJ/mol	339.50	NIST Webbook
hvapt	34.50	kJ/mol	317.50	NIST Webbook
rfi	1.39713		298.15	KDB
rfi	1.39992		293.15	Excess Volume of the 1-Propanol + 1-Alkene Systems in Terms of an Equation of State with Association
rhoI	697.00	kg/m ³	293.00	KDB
sfust	82.54	J/mol×K	153.40	NIST Webbook
srf	0.02	N/m	298.20	KDB
tcondl	0.11	W/m×K	320.83	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.12	W/m×K	297.95	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons

tcondl	0.11	W/m×K	320.47	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.12	W/m×K	297.71	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.11	W/m×K	321.08	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.13	W/m×K	262.75	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.13	W/m×K	262.46	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons

tcondl	0.12	W/m×K	297.36	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.13	W/m×K	281.03	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.13	W/m×K	280.80	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.13	W/m×K	280.48	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.13	W/m×K	262.97	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.43101e+01
Coeff. B	-3.15735e+03
Coeff. C	-4.10140e+01
Temperature range (K), min.	266.18
Temperature range (K), max.	391.88

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C \cdot \ln(T) + D \cdot T^2$
Coeff. A	8.49146e+01
Coeff. B	-7.03286e+03
Coeff. C	-1.05363e+01
Coeff. D	8.19459e-06
Temperature range (K), min.	154.27
Temperature range (K), max.	537.29

Datasets

Mass density, kg/m³

Temperature, K - Liquid	Pressure, kPa - Liquid	Mass density, kg/m ³ - Liquid
283.53	100.00	705.5
283.53	500.00	705.9
283.53	1000.00	706.4
283.53	3000.00	708.2
283.53	5000.00	710.0
283.53	10000.00	714.3
283.52	15000.00	718.3
283.52	20000.00	722.2
283.52	25000.00	725.9

283.52	30000.00	729.4
283.52	35000.00	732.9
283.52	40000.00	736.1
283.53	45000.00	739.3
283.53	50000.00	742.4
283.52	55000.00	745.3
283.53	60000.00	748.2
283.54	70000.00	753.8
283.53	80000.00	759.0
283.53	90000.00	763.9
283.54	100000.00	768.7
293.45	100.00	697.0
293.45	500.00	697.4
293.45	1000.00	697.9
293.46	3000.00	699.9
293.45	5000.00	701.8
293.46	10000.00	706.4
293.46	15000.00	710.7
293.45	20000.00	714.8
293.45	25000.00	718.7
293.45	30000.00	722.4
293.45	35000.00	726.0
293.46	40000.00	729.4
293.46	45000.00	732.8
293.46	50000.00	736.0
293.45	55000.00	739.0
293.45	60000.00	742.0
293.45	70000.00	747.8
293.45	80000.00	753.2
293.45	90000.00	758.3
293.45	100000.00	763.1
303.37	100.00	688.4
303.37	500.00	688.9
303.38	1000.00	689.5
303.38	3000.00	691.6
303.38	5000.00	693.6
303.38	10000.00	698.5
303.38	15000.00	703.1
303.38	20000.00	707.4
303.38	25000.00	711.5
303.38	30000.00	715.4
303.38	35000.00	719.2
303.38	40000.00	722.8
303.38	45000.00	726.2

303.38	50000.00	729.5
303.37	55000.00	732.8
303.38	60000.00	735.9
303.38	70000.00	741.8
303.38	80000.00	747.4
303.38	90000.00	752.6
303.37	100000.00	757.7
313.29	100.00	680.6
313.30	500.00	681.1
313.31	1000.00	681.8
313.31	3000.00	684.0
313.30	5000.00	686.2
313.31	10000.00	691.3
313.31	15000.00	696.3
313.30	20000.00	700.9
313.30	25000.00	705.2
313.30	30000.00	709.3
313.30	35000.00	713.3
313.30	40000.00	717.0
313.30	45000.00	720.6
313.30	50000.00	724.0
313.30	55000.00	727.4
313.30	60000.00	730.6
313.30	70000.00	736.8
313.30	80000.00	742.6
313.30	90000.00	748.0
313.30	100000.00	753.1
323.18	100.00	670.5
323.18	500.00	671.0
323.18	1000.00	671.6
323.18	3000.00	674.1
323.19	5000.00	676.4
323.18	10000.00	682.0
323.19	15000.00	687.1
323.19	20000.00	692.0
323.18	25000.00	696.6
323.18	30000.00	700.9
323.18	35000.00	705.0
323.18	40000.00	708.9
323.18	45000.00	712.7
323.18	50000.00	716.3
323.18	55000.00	719.7
323.18	60000.00	723.1
323.18	70000.00	729.6

323.18	80000.00	735.5
323.19	90000.00	741.1
323.19	100000.00	746.4
333.04	100.00	661.5
333.04	500.00	662.0
333.04	1000.00	662.7
333.05	3000.00	665.3
333.05	5000.00	667.9
333.05	10000.00	673.8
333.05	15000.00	679.3
333.05	20000.00	684.5
333.05	25000.00	689.3
333.05	30000.00	693.8
333.05	35000.00	698.1
333.05	40000.00	702.2
333.05	45000.00	706.2
333.05	50000.00	709.9
333.05	55000.00	713.5
333.05	60000.00	717.0
333.05	70000.00	723.7
333.05	80000.00	729.9
333.05	90000.00	735.7
333.05	100000.00	741.1
342.91	100.00	652.7
342.91	500.00	653.3
342.91	1000.00	654.0
342.91	3000.00	656.9
342.92	5000.00	659.6
342.92	10000.00	666.0
342.91	15000.00	671.8
342.92	20000.00	677.4
342.92	25000.00	682.4
342.91	30000.00	687.1
342.91	35000.00	691.7
342.92	40000.00	696.0
342.92	45000.00	700.1
342.92	50000.00	703.9
342.92	55000.00	707.7
342.92	60000.00	711.3
342.92	70000.00	718.3
342.92	80000.00	724.6
342.92	90000.00	730.6
342.92	100000.00	736.2
352.80	100.00	644.3

352.80	500.00	644.9
352.81	1000.00	645.7
352.81	3000.00	648.8
352.81	5000.00	651.6
352.81	10000.00	658.4
352.81	15000.00	664.7
352.81	20000.00	670.5
352.81	25000.00	675.8
352.81	30000.00	680.9
352.81	35000.00	685.6
352.80	40000.00	690.0
352.80	45000.00	694.3
352.80	50000.00	698.4
352.81	55000.00	702.3
352.81	60000.00	706.0
352.80	70000.00	713.2
352.80	80000.00	719.7
352.80	90000.00	725.9
352.80	100000.00	731.7
362.68	100.00	633.6
362.68	500.00	634.3
362.69	1000.00	635.0
362.69	3000.00	638.5
362.69	5000.00	641.7
362.70	10000.00	649.1
362.70	15000.00	655.8
362.69	20000.00	661.9
362.70	25000.00	667.6
362.69	30000.00	672.8
362.69	35000.00	677.8
362.69	40000.00	682.5
362.69	45000.00	687.0
362.69	50000.00	691.2
362.69	55000.00	695.2
362.69	60000.00	699.1
362.69	70000.00	706.6
362.69	80000.00	713.4
362.69	90000.00	719.7
362.68	100000.00	725.7

Reference

<https://www.doi.org/10.1021/acs.jced.8b00229>

Pressure, kPa

Temperature, K

Mass density, kg/m³

98.00	298.15	694.51
98.00	303.15	689.57
98.00	312.83	680.92
98.00	322.39	672.17
98.00	327.49	668.07
98.00	340.21	655.95
98.00	354.73	643.5
98.00	360.03	638.93
24510.00	298.15	718.23
24510.00	303.15	715.0
24510.00	327.47	697.97
24510.00	360.06	672.86
24510.00	392.79	646.48
24510.00	424.11	619.97
24510.00	452.35	595.84
24510.00	473.70	578.48
49030.00	298.15	734.7
49030.00	303.15	733.1
49030.00	327.49	718.4
49030.00	359.96	699.31
49030.00	392.68	676.29
49030.00	424.17	653.79
49030.00	452.34	628.89
49030.00	473.56	612.5
98060.00	298.15	765.58
98060.00	303.15	761.82
98060.00	327.48	746.71
98060.00	359.87	730.37
98060.00	392.74	714.89
98060.00	424.17	697.03
98060.00	452.25	676.86
98060.00	473.47	665.45
147100.00	298.15	783.57
147100.00	303.15	780.46
147100.00	327.63	767.87
147100.00	359.74	750.76
147100.00	392.61	734.09
147100.00	424.04	717.45
147100.00	452.28	702.95
147100.00	473.33	692.3
196130.00	298.15	800.85
196130.00	303.15	797.46
196130.00	327.63	786.42
196130.00	359.75	773.85

196130.00	392.46	758.9
196130.00	423.82	745.35
196130.00	452.22	733.49
196130.00	473.28	723.12
245160.00	298.15	816.79
245160.00	303.15	815.3
245160.00	327.67	805.58
245160.00	359.63	791.61
245160.00	392.40	776.73
245160.00	424.07	760.78
245160.00	452.27	750.38
245160.00	473.35	737.15

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Legend

af:	Acentric Factor
aiqt:	Autoignition Temperature
ap:	Aniline Point
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
dm:	Dipole Moment
dvisc:	Dynamic viscosity
fl:	Lower Flammability Limit
fpo:	Flash Point (Open Cup Method)
gf:	Standard Gibbs free energy of formation
hcg:	Heat of Combustion, Gross form
hcn:	Heat of Combustion, Net Form
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rfi:	Refractive Index
rhoc:	Critical density
rhof:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
sfust:	Entropy of fusion at a given temperature
sl:	Liquid phase molar entropy at standard conditions
srf:	Surface Tension
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tcondl:	Liquid thermal conductivity
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature

vc: Critical Volume
zc: Critical Compressibility
zra: Rackett Parameter

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